Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 08:41 am GMT

PDB ID	:	2JDV
Title	:	Structure of PKA-PKB chimera complexed with A-443654
Authors	:	Davies, T.G.; Verdonk, M.L.; Graham, B.; Saalau-Bethell, S.; Hamlett, C.C.F.; Mchardy, T.; Collins, I.; Garrett, M.D.; Workman, P.; Woodhead, S.J.; Jhoti, H.; Barford, D.
Deposited on	:	2007-01-12
Resolution	:	2.08 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

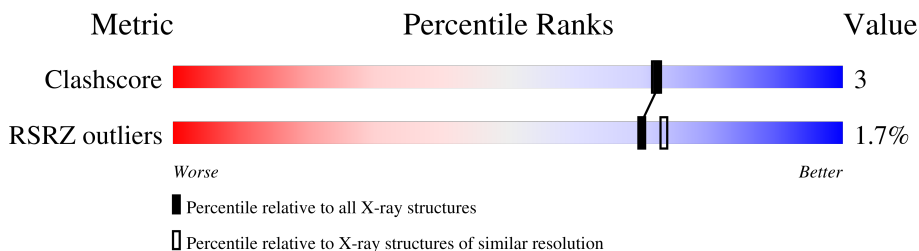|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	FAILED
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		3
RSRZ outliers		1.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6738 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	351	2% ▮ 87% 8% •
2	I	20	85% 10% 5%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 3268 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CAMP-DEPENDENT PROTEIN KINASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	336	Total 2778	C 1800	N 466	O 500	P 2	S 10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	104	THR	VAL	engineered mutation	UNP P00517
A	123	ALA	VAL	engineered mutation	UNP P00517
A	173	MET	LEU	engineered mutation	UNP P00517
A	181	LYS	GLN	engineered mutation	UNP P00517

- Molecule 2 is a protein called CAMP-DEPENDENT PROTEIN KINASE INHIBITOR ALPHA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	20	Total 157	C 94	N 32	O 31	0	0	0

- Molecule 3 is (2S)-1-(1H-INDOL-3-YL)-3-{[5-(3-METHYL-1H-INDAZOL-5-YL)PYRIDIN-3-YL]OXY}PROPAN-2-AMINE (three-letter code: L20) (formula: $C_{24}H_{23}N_5O$).

L20
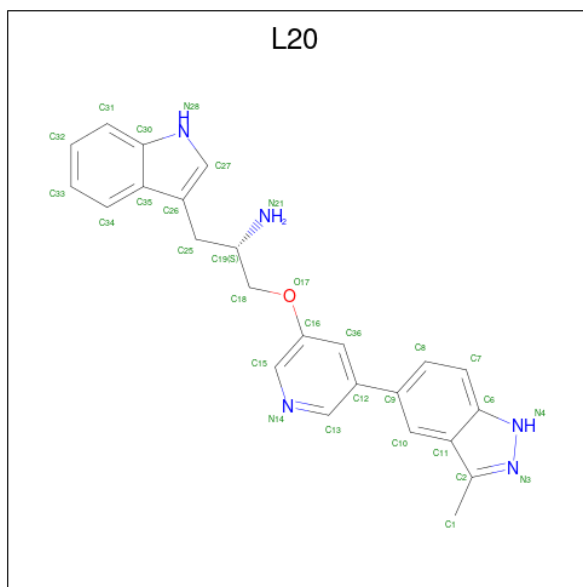
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	30	24	5	1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	271	271	271	0	0
4	I	32	Total	O	0	0
			32	32		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CAMP-DEPENDENT PROTEIN KINASE
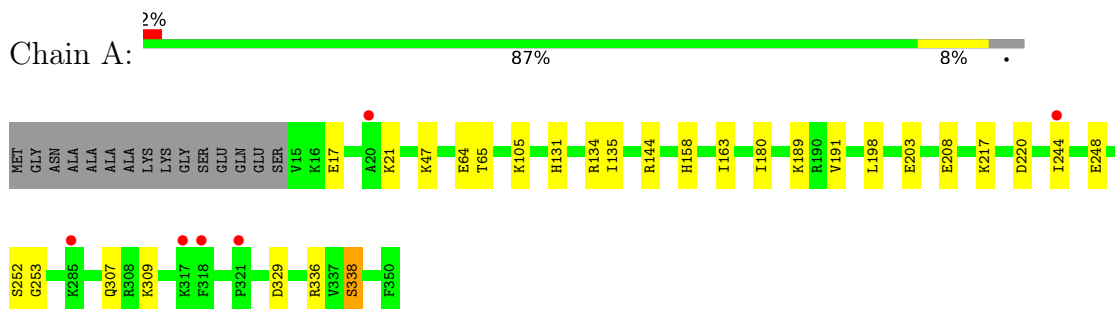
• Molecule 2: CAMP-DEPENDENT PROTEIN KINASE INHIBITOR ALPHA
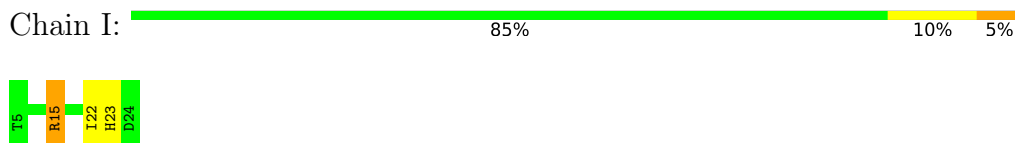
4 Data and refinement statistics (i)

Xtriage (Phenix) failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.81Å 74.79Å 80.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.40 – 2.08 35.40 – 2.08	Depositor EDS
% Data completeness (in resolution range)	93.6 (35.40-2.08) 93.5 (35.40-2.08)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019F	Depositor
R, R_{free}	0.206 , 0.276 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3268	wwPDB-VP
Average B, all atoms (Å²)	27.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: L20, TPO, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.74	0/2828	0.76	5/3807 (0.1%)
2	I	0.84	0/159	1.04	2/212 (0.9%)
All	All	0.74	0/2987	0.78	7/4019 (0.2%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	15	ARG	NE-CZ-NH2	-7.90	116.35	120.30
2	I	15	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	A	134	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	208	GLU	CB-CA-C	-5.65	99.10	110.40
1	A	134	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	144	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	180	ILE	CB-CA-C	-5.01	101.57	111.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2778	0	2758	18	0
2	I	157	0	146	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	30	0	23	0	0
4	A	271	0	0	1	0
4	I	32	0	0	2	0
All	All	3268	0	2927	20	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:HIS:O	1:A:135:ILE:HD12	1.84	0.77
1:A:64:GLU:HG2	1:A:65:THR:HG23	1.81	0.63
1:A:158:HIS:HE1	1:A:220:ASP:OD2	1.83	0.61
1:A:336:ARG:NH2	1:A:338:SEP:O1P	2.34	0.58
1:A:64:GLU:CG	1:A:65:THR:HG23	2.35	0.57
2:I:15:ARG:NH2	4:I:2011:HOH:O	2.38	0.57
1:A:189:LYS:HE2	1:A:191:VAL:CG1	2.38	0.54
1:A:105:LYS:HG3	4:A:2098:HOH:O	2.10	0.52
1:A:198:LEU:HD22	2:I:22:ILE:HD11	1.90	0.52
1:A:244:ILE:O	1:A:248:GLU:HG3	2.09	0.51
2:I:23:HIS:NE2	4:I:2031:HOH:O	2.33	0.51
1:A:189:LYS:HE2	1:A:191:VAL:HG11	1.96	0.47
1:A:189:LYS:HG2	1:A:191:VAL:HG13	1.98	0.46
1:A:17:GLU:HG2	1:A:21:LYS:NZ	2.30	0.46
1:A:189:LYS:CE	1:A:191:VAL:CG1	2.94	0.45
1:A:203:GLU:OE2	2:I:15:ARG:HD3	2.19	0.43
1:A:252:SER:OG	1:A:253:GLY:N	2.52	0.42
1:A:163:ILE:HG12	1:A:217:LYS:HG2	2.01	0.42
1:A:307:GLN:HE21	1:A:309:LYS:HD2	1.84	0.42
1:A:47:LYS:NZ	1:A:329:ASP:OD1	2.48	0.40

There are no symmetry-related clashes.

5.3   Torsion angles (i)

5.3.1   Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2   Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3   RNA (i)

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
1	TPO	A	197	1	8,10,11	0.90	0	10,14,16	0.97	0
1	SEP	A	338	1	8,9,10	1.41	1 (12%)	8,12,14	2.16	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	197	1	-	1/9/11/13	-
1	SEP	A	338	1	-	3/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	338	SEP	P-O1P	3.01	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	SEP	OG-CB-CA	5.23	113.24	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	338	SEP	OG-P-O1P	2.11	112.38	106.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	197	TPO	O-C-CA-CB
1	A	338	SEP	N-CA-CB-OG
1	A	338	SEP	CA-CB-OG-P
1	A	338	SEP	CB-OG-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	338	SEP	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	L20	A	1351	-	30,34,34	1.29	2 (6%)	29,48,48	1.62	7 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	L20	A	1351	-	-	2/8/13/13	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1351	L20	C1-C2	-3.75	1.47	1.50
3	A	1351	L20	C25-C19	2.33	1.57	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1351	L20	C1-C2-N3	2.99	126.22	119.65
3	A	1351	L20	C11-C10-C9	-2.91	118.54	122.01
3	A	1351	L20	C13-N14-C15	2.90	119.33	116.87
3	A	1351	L20	O17-C18-C19	-2.88	101.94	108.29
3	A	1351	L20	C8-C7-C6	-2.76	115.70	120.76
3	A	1351	L20	C18-O17-C16	2.17	122.52	117.93
3	A	1351	L20	C25-C26-C27	-2.12	125.35	127.97

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1351	L20	C36-C16-O17-C18
3	A	1351	L20	C15-C16-O17-C18

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand L20 A 1351

Bond lengths

Bond angles

Torsions

Rings
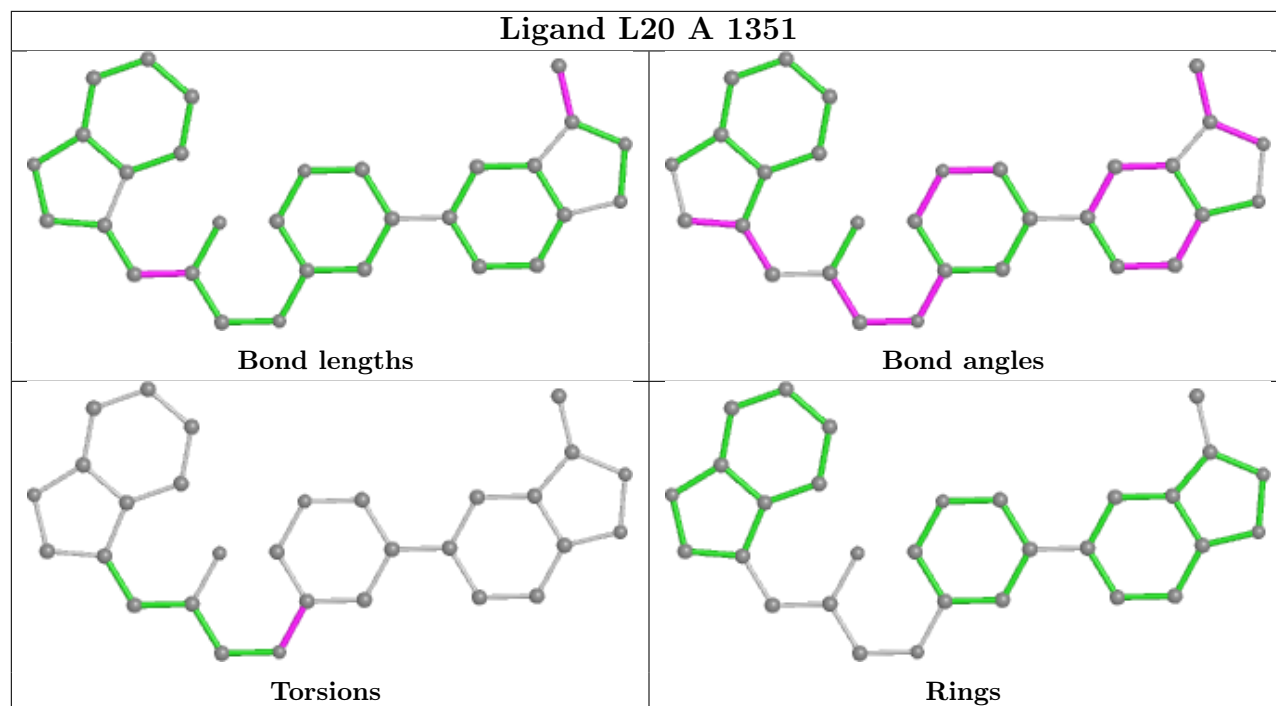
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	334/351 (95%)	0.13	6 (1%) 68	71	13, 24, 44, 73	0
2	I	20/20 (100%)	-0.06	0 100	100	17, 21, 57, 60	0
All	All	354/371 (95%)	0.12	6 (1%) 70	73	13, 24, 45, 73	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	PHE	6.1
1	A	321	PRO	4.5
1	A	317	LYS	2.6
1	A	244	ILE	2.6
1	A	285	LYS	2.4
1	A	20	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	A	338	10/11	0.97	0.12	31,34,37,39	0
1	TPO	A	197	11/12	0.98	0.09	13,16,17,19	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	L20	A	1351	30/30	0.96	0.15	13,18,23,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.